group scatterers in lieu of individual atomic ones improves the efficiency by almost an order of magnitude. We are currently testing the method on oligonucleotide and protein structures.

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An Analytical Method for Studying the Variation of the Interfacial Symmetry Due to Relative Displacements of the Bicrystal Components

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Abstract

This paper investigates changes of the bicrystal symmetry caused by rigid-body relaxation. Analytical expressions are derived for the determination of the symmetry of a bicrystal, or, more generally, of a binary composite, corresponding to a particular relative displacement of its components. Such displacements can change the point and/or space symmetry of the composite either by compressing symmetry operations or by transforming symmorphic symmetry operations to their nonsymmorphic counterparts, or *vice versa*. In the latter case the relative displacements have a well defined magnitude and direction and it is shown that the composite space groups associated with these displacements correspond to a new type of subgroups of space groups. These subgroups, although having the same unit cell as the original space group, are similar to the *klassengleiche* subgroups in the sense that the descent in symmetry has affected the translations in the unit cell of the original group. Furthermore, it is pointed out that the reduction of symmetry due to relative displacements is accomplished by a multiplicity of crystallographically equivalent ways and that their number and interrelation depends on the space symmetry of the original composite.

1. Introduction

The crystallographic framework of planar grain boundaries was recently discussed by Pond & Bollmann (1979). Their considerations, enabling the description of the interfacial symmetry, were based on the introduction of the bicrystal which is defined as the system of the two adjacent crystals containing the planar interface. The starting point of the methodology of Pond & Bollmann, which was subsequently extended by Vlachavas (1980) and Pond &

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Vlachavas (1983), is the following idealized construction of a bicrystal.

We begin by interpenetrating the two lattice complexes corresponding to the two crystals of the bicrystal so that they have a common origin and are in complete coincidence. For convenience, one lattice complex is designated black and the other white (Pond & Bollmann, 1979). The desired relative orientation and position of the bicrystal components is then obtained by: (i) causing the black lattice complex to undergo a rotation R while keeping the white lattice complex fixed in space, and (ii) translating the black complex by $\mathbf{t}$ with respect to the white complex. The interpenetrating configuration of black and white lattice complexes thus obtained is called, following Vlachavas (1980), the dichromatic complex.

Having obtained the dichromatic complex for the desired R and $\mathbf{t}$ we are now in a position to create the bicrystal. We start by introducing a mathematical plane into the dichromatic complex in the orientation and position of the chosen interface. The bicrystal is then obtained by locating atoms at the positions of the black lattice complex on one side of the interface and at the positions of the white lattice complex on the other side.

This procedure for manufacturing a bicrystal can be successfully applied to express the bicrystal symmetry in terms of the space group and the relative orientation and position of the crystals adjoining the interface. The relationship between the bicrystal symmetry and the space group of the adjacent crystals was investigated by Pond & Vlachavas (1983); the variation of bicrystal symmetry with changes in the relative orientation of the component crystals can be obtained by the treatment described by Vlachavas (1984). Thus, one of the questions that remains to be answered is: 'how does the symmetry of the dichromatic complex or the bicrystal vary when the black lattice complex undergoes a shift with respect to the white lattice complex?'. These symmetry changes are the objective of the analytical treatment developed in this paper. The proposed approach can be applied equally well to study the symmetry variation with displacement of either the dichromatic complexes or bicrystals. Consequently, in our considerations we will refer to the more general case of a dichromatic composite characterized by a specific combination of two identical components. These components may, in general, have zero-, one-, two- or three-dimensional periodicity.

The analytical treatment proposed in this paper also enables the determination of the interrelationship of certain rigid-body relaxed interfaces. Computer simulation (see *e.g.* Smith, Vitek & Pond, 1977; Pond, Smith & Vitek, 1979) and transmission electron microscopy observations (Pond & Vitek, 1977; Pond, 1979) indicate that the energetically favourable structures of coincidence-site-lattice grain boundaries are characterized by specific relative translations. Such rigid-body displacements lead, as pointed out by Pond (1977), to a multiplicity of possible configurations that can exist for a given coincidence-site-lattice grain boundary. The number and disposition of rigid-body relaxed interfaces are obtained by analysing the bicrystal symmetry variation with displacement according to the treatment developed in this paper.

As mentioned above, one of the components of the dichromatic composite is regarded white and the other black. Thus, the point and/or space group of the dichromatic composite is expressed by using two-coloured symmetry formulation (see *e.g.* Shubnikov & Koptsik, 1974). In this way, symmetry relationships between the two components are described by colour-reversing symmetry operations, whereas the symmetry between parts of the same component corresponds to ordinary symmetry operations. The symbols of symmetry operations, elements and groups used in this paper are consistent with the notation outlined by Vlachavas (1984).

The parallel displacement of, say, the black component with respect to the white one changes the point and/or space symmetry of the dichromatic composite. The variation of the point symmetry with relative displacement is examined in part I of the paper while in part II we consider the more general case of periodic composites. Though this method involves a slight expansion and some repetition of the work, for reasons of clarity it appears preferable to a direct consideration of the more general problem and a subsequent deduction of the simpler one as a particular case.

2. Part I: Point-symmetry variation

For studying the symmetry variation of a dichromatic composite its white component is considered fixed in space and is used as the reference component. Any relative displacement between the two components is introduced by the appropriate translation of the black component. This translation is represented by the vector which connects the origin of the orthogonal coordinate system of the white component to the origin of the black coordinate system. This vector expressed relative to the white coordinate system is $\mathbf{t} = \alpha\mathbf{i} + \beta\mathbf{j} + \gamma\mathbf{k}$, where $\mathbf{i}, \mathbf{j}, \mathbf{k}$ are the unit vectors along the x, y and z axes, respectively, and will be denoted by $\mathbf{t} = (\alpha, \beta, \gamma)$.

If the black component is displaced away from its original position, the geometrical relationship and, hence, the symmetry between the two components changes. As an example, let the dichromatic composite in Fig. 1(a) be obtained by superposing two rectangles which are rotated relative to one another by 90°. The symmetry of the composite (on a one-sided plane) is $4'mm'$. Next we displace the black rectangle by $\mathbf{t}=(x, 0, 0)$, *i.e.* by an arbitrary amount along the x axis, and we see (Fig. 1b) that the symmetry of the composite is reduced to m.

2.1. *Subgroup relations in the point-symmetry variation*

It is seen by comparing the composites in Figs. 1(a) and (b) that the relative displacement destroys some of the symmetry operations of the original composite while it conserves others and yields, consequently, a composite with lower symmetry. This is so, however, only when the original composite is holosymmetric, *i.e.* when the original composite exhibits the highest possible symmetry which can be created by the superposition of two given components in a given misorientation relationship.*

For finite components and for a particular misorientation the unique translational position of the two components leading to the holosymmetric composite corresponds to $\mathbf{t}=\mathbf{0}$. This is so because, as pointed out by Vlachavas (1980), the dichromatic composite has the common symmetry of the individual components augmented by the operations of rotation and translation which describe their mutual position. When the components have common origin they possess the maximum number of common symmetry elements for the given misorientation and, consequently, the composite exhibits the highest possible symmetry.

In what follows the composite with $\mathbf{t}=\mathbf{0}$ is taken to be always holosymmetric, unless specifically stated to be otherwise. In this case the point symmetry of the composite after any displacement is a subgroup of the original point group. First of all, it is a group by virtue of the restrictions placed upon the conservation of its elements. No product of elements in the set can be unrelated to the particular geometrical relationship of the two components, and all elements of the initial composite related to this relationship are included in the set. Secondly, it is a subgroup because in displacing the black component symmetry elements are removed but not added as long as the initial composite is holosymmetric.

Having established the relationship between the composite point groups before and after displacement an analytical approach for investigating the point symmetry variation can be derived. For this the colour-reversing and ordinary symmetry operations are considered separately.

* The rotation of the black component relative to the white one is called the misorientation relationship of the two components (or misorientation for short).

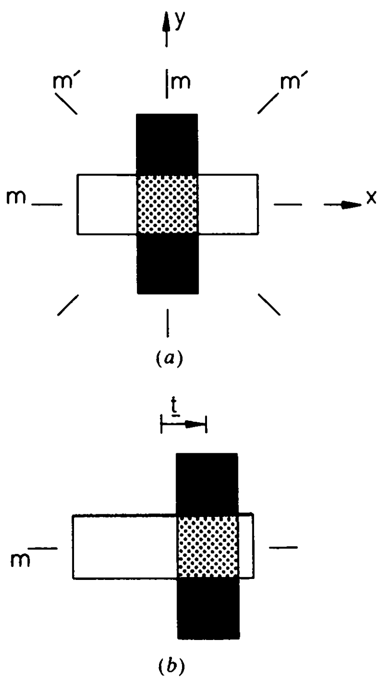

Fig. 1. The variation of the point symmetry with displacement. The original composite in (a) is obtained by the superposition of a white and a black rectangle which are relatively rotated by 90°; its symmetry is $4'mm'$. When the black component is displaced by $\mathbf{t}=(x, 0, 0)$ the composite symmetry is reduced to m(b). The coordinate system is shown in (a); the z axis is out of the plane of the paper.

2.2. *Conservation of colour-reversing symmetry operations*

The colour-reversing symmetry operations of the dichromatic composite arise by geometrical relationships between the white and black components. Thus, any displacement $\mathbf{t}$ which does not alter a particular relationship conserves the respective operation, which, however, is shifted by $\mathbf{t}/2$. Let us consider the following example. A dichromatic composite is obtained by superposing two rectangles in such a way that their long sides are coincident (Fig. 2a). The symmetry of the composite, which is not holosymmetric, is $2'mm'$. Next, we displace the black rectangle by $\mathbf{t}=(x, 0, 0)$ and we see (Fig. 2b) that the mirror plane m' has been shifted by $(x/2, 0, 0)$ relative to its original position.

When the black component is displaced by $\mathbf{t}$ the origin of the coordinate system has to be displaced by $\mathbf{t}/2$ in order to retain the form of the symmetry-operation matrix representations (this coordinate system is called the 'displaced coordinate system'). Alternatively stated, it can be considered that the black component is displaced by $\mathbf{t}/2$ and at the same time the white component by $-\mathbf{t}/2$. In this case the conserved symmetry elements remain in their initial positions and, hence, they are expressed relative to the original coordinate system.

Let S_c be a colour-reversing symmetry operation which is conserved by the displacement $\mathbf{t}$. Since S_c is present in the original composite there is at least a pair of points belonging to the white and black components–their positions in the original composite are denoted by $\mathbf{r}_w$ and $\mathbf{r}_b$, respectively – for which

$$S_c\mathbf{r}_w = \mathbf{r}_b.$$

If the white and black components are displaced by $-\mathbf{t}/2$ and $\mathbf{t}/2$, the positions of the above points relative to the original coordinate system become $\mathbf{r}_w - \mathbf{t}/2$ and $\mathbf{r}_b + \mathbf{t}/2$, respectively. The symmetry relationship of the two points is now expressed by

$$S_c(\mathbf{r}_w - \mathbf{t}/2) = \mathbf{r}_b + \mathbf{t}/2.$$

Consequently, a colour-reversing symmetry operation in the dichromatic composite is conserved at its original position only for displacements which satisfy the relation

$$S_c(-\mathbf{t}/2) = \mathbf{t}/2, \quad (1)$$

where the displacement $\mathbf{t}/2$ is expressed relative to the coordinate system of the original composite (*i.e.* the composite before displacement). Equivalently, (1) gives the displacement $\mathbf{t}$ of the black component which conserves the colour-reversing operation S_c. However, in this case S_c is shifted by $\mathbf{t}/2$ from its original position.

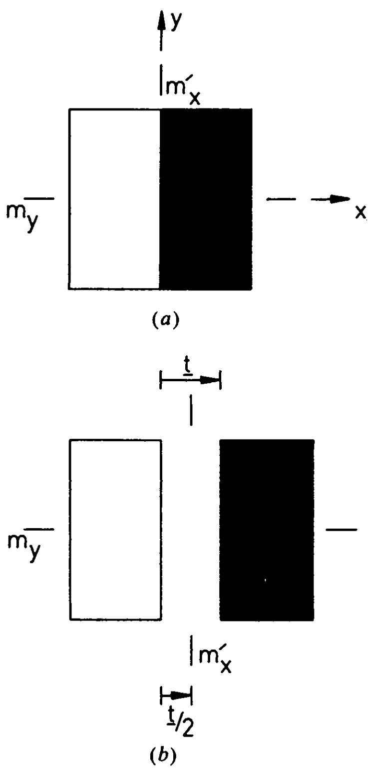

Fig. 2. The shift of symmetry elements with displacement. The original composite is shown in (*a*) and has symmetry $2'm'm$. In (*b*) the black rectangle is shifted by $\mathbf{t} = (x, 0, 0)$ and the composite symmetry is again $2'm'm$. However, the mirror m'_x is shifted by $\mathbf{t}/2 = (x/2, 0, 0)$ from its original position. The z axis of the coordinate system is out of the plane of the paper; the x and y axes are indicated in (*a*).

2.3. *Conservation of ordinary symmetry operations*

Ordinary symmetry operations in the dichromatic composite arise by the coincidence of identical operations* of the two components (see Vlachavas, 1984) and, consequently, a displacement $\mathbf{t}$ conserves an ordinary symmetry operation only if it leaves them in coincidence. Referring to Fig. 2, for an example, we note that the mirror m_y occurs in the dichromatic composite because of the coincidence of the mirror planes of the individual components. Also, we note that the displacement $\mathbf{t} = (x, 0, 0)$ is parallel to m_y and, hence, it conserves this mirror plane at its original position.

Let S_o be an ordinary symmetry operation which is conserved when the two components are displaced relative to each other by $\mathbf{t}$. In the original composite there is at least a pair of white points, $\mathbf{r}_w$ and $\mathbf{r}'_w$, as well as a pair of black points, $\mathbf{r}_b$ and $\mathbf{r}'_b$, for which

$$S_o\mathbf{r}'_w = \mathbf{r}_w \quad \text{and} \quad S_o\mathbf{r}'_b = \mathbf{r}_b.$$

After displacement $\mathbf{t}$ the positions of the points in the white component become $\mathbf{r}_w - \mathbf{t}/2$ and $\mathbf{r}'_w - \mathbf{t}/2$ and those in the black component $\mathbf{r}_b + \mathbf{t}/2$ and $\mathbf{r}'_b + \mathbf{t}/2$, respectively. Therefore, the symmetry relationships of the two points are given by

$$S_o(\mathbf{r}'_w - \mathbf{t}/2) = \mathbf{r}_w - \mathbf{t}/2 \quad \text{and} \quad S_o(\mathbf{r}'_b + \mathbf{t}/2) = \mathbf{r}_b + \mathbf{t}/2.$$

Consequently, an ordinary symmetry operation is conserved by a displacement only if

$$S_o(\mathbf{t}/2) = \mathbf{t}/2, \quad (2)$$

where, again, the displacement $\mathbf{t}/2$ is expressed relative to the coordinate system of the original composite.

2.4. *Example of point-symmetry variation*

The application of the relations derived in the foregoing sections is now demonstrated with reference to a particular example. Let both the white and black components be non-periodic† with symmetry $4/mmm$ and let these be superposed so the obtained composite has symmetry $4/mm'm'$. This black–white point group contains the following symmetry operations:

ordinary operations:

$$1, 4^1_{001}, 4^3_{001}, 2^1_{001}, i, \bar{4}^1_{001}, \bar{4}^3_{001}, s_{001}$$

colour-reversing operations:

$$2^{1'}_{100}, 2^{1'}_{010}, 2^{1'}_{110}, 2^{1'}_{\bar{1}10}, s'_{100}, s'_{010}, s'_{110}, s'_{\bar{1}10}.$$

*This implies, of course, that the symmetry operations of both the white and black point groups are expressed relative to the same coordinate system.

†This implies that point symmetry only is taken into account; the method is, however, identically applied for studying the point-symmetry variation of periodic composites.

Table 1. *Subgroups of the black–white point group* $4/mm'm'$ (*see Ascher & Janner*, 1965)

All the subgroups are included in the table; from the total 35 subgroups only 19 are crystallographically non-equivalent.

No.	Subgroup	1	4^1_{001}	4^3_{001}	2^1_{001}	$2^{1'}_{100}$	$2^{1'}_{010}$	$2^{1'}_{110}$	$2^{1'}_{\bar{1}10}$	i	$\bar{4}^1_{001}$	$\bar{4}^3_{001}$	s_{001}	s'_{100}	s'_{010}	s'_{110}	$s'_{\bar{1}10}$
1	$4/mm'm'$	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×
2	$\bar{4}2'm'$	×			×	×	×				×	×				×	×
3	$\bar{4}2'm'$	×			×			×	×		×	×		×	×		
4	$4m'm'$	×	×	×	×									×	×	×	×
5	$42'2'$	×	×	×	×	×	×	×	×								
6	$4/m$	×	×	×	×					×	×	×	×				
7	$\bar{4}$	×			×						×	×					
8	4	×	×	×	×												
9	$m'm'm$	×			×	×	×			×			×	×	×		
10	$m'm'm$	×			×			×	×	×			×			×	×
11	$m'm2'$	×				×							×		×		
12	$m'm2'$	×					×						×	×			
13	$m'm2'$	×						×					×				×
14	$m'm2'$	×							×				×			×	
15	$2'/m'$	×				×				×				×			
16	$2'/m'$	×					×			×					×		
17	$2'/m'$	×						×		×						×	
18	$2'/m'$	×							×	×							×
19	$2/m$	×			×					×			×				
20	$m'm'2$	×			×									×	×		
21	$m'm'2$	×			×											×	×
22	$2'2'2$	×			×	×	×										
23	$2'2'2$	×			×			×	×								
24	$\bar{1}$	×								×							
25	m'	×												×			
26	m'	×													×		
27	m'	×														×	
28	m'	×															×
29	$2'$	×				×											
30	$2'$	×					×										
31	$2'$	×						×									
32	$2'$	×							×								
33	m	×											×				
34	2	×			×												
35	1	×															

The z axis of the orthogonal coordinate system used for expressing the symmetry operations and the displacements is along the fourfold axis. The x and y axes, on the other hand, coincide with two mutually perpendicular twofold axes of the point group.

The symmetry $4/mm'm'$ corresponds to the holosymmetric composite created by the given components in the given misorientation. Consequently, the symmetry of the composites after displacement will correspond to one of the subgroups of $4/mm'm'$ given in Table 1.

The next stage in the procedure is to determine the displacements for which each of the symmetry operations of $4/mm'm'$ is invariant. Colour-reversing operations are conserved by the displacements obtained as solutions of (1) (Table 2). On the other hand, the displacements conserving ordinary operations are, according to (2), those in Table 3. In applying the results of Tables 2 and 3 it must be borne in mind that they correspond to symmetry operations. The displacements conserving a particular symmetry element are those which leave all the symmetry operations associated to this element invariant. The ordinary fourfold axis, for example, involves the presence of the four symmetry operations 1, 4^1_{001}, 2^1_{001}, 4^3_{001}. All these operations are conserved for displacements parallel to the z axis and, hence, the fourfold ordinary axis is conserved by $\mathbf{t}=(0,0,z)$.

Attention is now focused on displacements leading to a composite with symmetry described by any one of the subgroups of the point group $4/mm'm'$. For this, each subgroup given in Table 1 is considered starting with those of higher symmetry. For each subgroup a displacement conserving all the group elements can be established.* Consider the subgroup $42'2'=\{1, 4^1_{001}, 2^1_{001}, 4^3_{001}, 2^{1'}_{100}, 2^{1'}_{010}, 2^{1'}_{110}, 2^{1'}_{\bar{1}10}\}$. The fourfold axis is conserved by a displacement $(0,0,z)$ whereas the axes $2^{1'}_{100}$, $2^{1'}_{010}$, $2^{1'}_{110}$, $2^{1'}_{\bar{1}10}$ are conserved by the displacements $(0,y,z)$, $(x,0,z)$, $(\bar{x},x,z)$, (x,x,z), respectively. Therefore, the only displacement conserving all the elements of $42'2'$ is of the form $\mathbf{t}=(0,0,z)$. Similar considerations give the displacements which conserve each of the remaining subgroups (Table 4). Since the point group of the composite for $\mathbf{t}\neq\mathbf{0}$ is restricted to be a subgroup of the point group $4/mm'm'$ and since all the subgroups were considered it is clear that Table 4 covers all the possible composites obtained from the original composite.

* It should be remembered that certain subgroups are conserved only for the displacement $\mathbf{t}=\mathbf{0}$ (see below).

Table 2. *Solutions of the equation $S_c(-\mathbf{t}/2)=\mathbf{t}/2$ for the colour-reversing symmetry operations of the black–white point group $4/mm'm'$*

Symmetry element S_c: Symbol	Symmetry element S_c: Matrix representation	Displacements conserving the symmetry element S_c (expressed relative to original coordinate system)
$2^{1'}_{100}$	$\begin{pmatrix} 1 & 0 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$(0, y, z)$
$2^{1'}_{010}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$(x, 0, z)$
$2^{1'}_{110}$	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$(\bar{x}, x, z)$
$2^{1'}_{\bar{1}10}$	$\begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	(x, x, z)
s'_{100}	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$(x, 0, 0)$
s'_{010}	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$(0, y, 0)$
s'_{110}	$\begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$(x, x, 0)$
$s'_{\bar{1}10}$	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$(\bar{x}, x, 0)$

Table 3. *Solutions of the equation $S_0(\mathbf{t}/2)=\mathbf{t}/2$ for the ordinary symmetry operations of the black–white point group $4/mm'm'$*

Symmetry element S_o: Symbol	Symmetry element S_o: Matrix representation	Displacements conserving the symmetry element S_o (expressed relative to ordinary coordinate system)
1	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	(x, y, z)
4^{1}_{001}	$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$(0, 0, z)$
4^{3}_{001}	$\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$(0, 0, z)$
2^{1}_{001}	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$(0, 0, z)$
i	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$(0, 0, 0)$
$\bar{4}^{1}_{001}$	$\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$(0, 0, 0)$
$\bar{4}^{3}_{001}$	$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$(0, 0, 0)$
s_{001}	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$(x, y, 0)$

When the displacements conserving the elements of a subgroup are determined the following must be kept in mind:

(*a*) since the (ordinary) identity operation is conserved by any displacement there is no need to account for this operation;

(*b*) certain subgroups are not invariant by displacements $\mathbf{t}\neq\mathbf{0}$; the subgroup $\bar{4}2'm'$, for example, is conserved by the displacement $\mathbf{t}=(0,0,0)$ only; and

(*c*) certain subgroups are formed by displacements which at the same time conserve another subgroup of higher symmetry.

The latter is a consequence of the conservation of various symmetry elements by the same displacement. For example, both subgroups $42'2'$ and 4 are formed by a displacement of the form $(0, 0, z)$. This happens when the two groups contain common elements, or, in other words, when the two groups are related by a subgroup/supergroup relationship. In such cases, however, the symmetry of the dichromatic composite is described by the highest-order subgroup (highest symmetry). This explains why the subgroup list must be considered in a sequence of decreasing group order.

2.5. *Equivalent composites*

It can be seen from Table 4 that composites with symmetry described by certain subgroups can be created by more than one crystallographically equivalent displacement.* This occurs whenever a subgroup adopts more than one crystallographically equivalent orientation in the point group of the original composite. The subgroup $m'm2'$, for instance, adopts four different orientations in $4/mm'm'$ differing over an angle of 45° about the fourfold axis; two of these orientations are not crystallographically equivalent. Only the first orientation is considered here, since the second case can be treated in exactly the same way. The two crystallographically equivalent subgroups $m'm2'$ (subgroups 11 and 12 in Table 4) are related by a symmetry operation, say 4^{1}_{001}, of the original composite. The

* It is possible that composites with identical symmetry can be created by crystallographically non-equivalent displacements. These cases, however, must be treated separately; this is a situation where the need to distinguish between crystallographically non-equivalent subgroups arises.

Table 4. *Point-symmetry variation of a composite with symmetry* $4/mm'm'$

Displacement expressed relative to original coordinate system	Point group No.*	Symbol
$(0, 0, 0)$	1	$4/mm'm'$
$(0, 0, z)$	5	$42'2'$
$(0, y, 0)$	11	$m'm2'$
$(x, 0, 0)$	12	$m'm2'$
$(\bar{x}, x, 0)$	13	$m'm2'$
$(x, x, 0)$	14	$m'm2'$
$(0, y, z)$	29	$2'$
$(x, 0, z)$	30	$2'$
$(\bar{x}, x, z)$	31	$2'$
(x, x, z)	32	$2'$
$(x, y, 0)$	33	m
(x, y, z)	35	1

*See Table 1.

same operation relates the displacements $\mathbf{t}_1 = (x, 0, 0)$ and $\mathbf{t}_2 = (0, y, 0)$ yielding the corresponding composites.

It can be stated that, in general, whenever an original composite contains point symmetry higher than 1 there exists a set of dichromatic composites, obtained from the original composite by displacements of the black component, which are related by the symmetry of the composite with $\mathbf{t} = \mathbf{0}$. The composites of such sets will be called 'equivalent composites'.

A crystallographic point group G can be decomposed into left cosets with respect to a subgroup H,

$$G = H + g_1 H + g_2 H + \ldots + g_{n-1} H,$$

where n is the index of H in G and g_i $(1 \le i \le n-1)$ is an operator of G which does not belong to H nor to any of the previous cosets. Each coset will correspond to a composite with $\mathbf{t} \neq \mathbf{0}$. The equivalent composites, having the same or crystallographically equivalent point symmetry, are related by the symmetry operations of the set $\{1, g_1, g_2, \ldots, g_{n-1}\}$. Thus, for the example mentioned above we have $G = 4/mm'm'$ and $H = m'm2'$ and the decomposition is

$$\begin{aligned}\{4/mm'm'\} &= \{m'm2'\} + 4^1_{001}\{m'm2'\} + 2^1_{001}\{m'm2'\} \\ &\quad + 4^3_{001}\{m'm2'\} \\ &= \{4\}\{m'm2'\}.\end{aligned}$$

Consequently, the equivalent composites with symmetry $m'm2'$ are obtained by the displacements $(x, 0, 0)$, $(0, x, 0)$, $(\bar{x}, 0, 0)$, $(0, \bar{x}, 0)$ which are also related by the symmetry operations of the group $4 = \{1, 4^1_{001}, 2^1_{001}, 4^3_{001}\}$.

It must be noticed that the set of symmetry operations relating equivalent composites is generally not unique; in the above case we have, for instance,

$$\begin{aligned}G &= H + 4^1_{001} H + 2^1_{001} H + 4^3_{001} H \\ &= H + s'_{110} H + s'_{\bar{1}10} H + 2^1_{001} H.\end{aligned}$$

A crystallographic point group may be decomposed into non-intersecting (except for the identity operator) subgroups, called direct factors, whose product* is the original group (Kurosh, 1955). Let the initial group G be decomposed into two factors, one of the subgroups is chosen to be the symmetry group H of the equivalent composites with $\mathbf{t} \neq \mathbf{0}$ and the other is designated G_g. This decomposition is not unique, however, so that, for a given G and H, G_g may be chosen in a number of ways $G_{g,i}$. Each such $G_{g,i}$ represents a set of symmetry operations, all independent of H, which relate equivalent composites. For the above considered case we have: $\{4/mm'm'\} = \{4\}\{m'm2'\} = \{m'm'2\}\{m'm2'\} = \{\bar{4}\}\{m'm2'\} = \ldots = \{2'/m'\}\{m'm2'\} = \{22'2'\}\{m'm2'\}$, but any of these decompositions gives the same set of displacements creating the equivalent composites with symmetry $m'm2'$.

2.6. *Conservation of point symmetry elements*

In this section we seek to determine the conditions for the conservation of symmetry elements. These conditions can be established if we recall that every symmetry element is associated with one or more symmetry operations.† The only symmetry element of order 1 is the identity (onefold ordinary axis) and, according to (2), there is no displacement which could destroy the symmetrical relationship of a point to itself.

Rule 1: The ordinary identity element is conserved by any relative displacement of the black and white components.

Symmetry elements of order greater than 1 are associated with either ordinary operations only or equal numbers of ordinary and colour-reversing operations. These symmetry elements are conserved by the displacements which leave all the correlative operations invariant. Consequently, a symmetry element of order n $(n > 1)$ is conserved by displacements determined from the solution of the system of equations

$$S_i\{(-1)^{\kappa}\mathbf{t}/2\} = \mathbf{t}/2,$$

where S_i $(i = 1, 2, \ldots, n)$ are the matrices representing the symmetry operations associated with the symmetry and $\kappa = 1$ for colour-reversing or $\kappa = 2$ for ordinary symmetry operations.

The symmetry elements of order 2 are $\bar{1}, 2, m, 1', \bar{1}', 2'$ and m'. Each of these elements is associated, except the identity, with only one ordinary or colour-reversing operation and, taking into account rule 1, the displacements conserving it are determined by (1) or (2) correspondingly. We have the following rules.

* A product is understood, in this context, as the sum of all products of the elements of the subgroups one by one.

† The number of symmetry operations coupled with a symmetry element is called the 'order of the element'.

Rule 2: No translation conserves the anti-identity operation.

Rule 3: The ordinary inversion centre is destroyed by any displacement whereas the anti-inversion centre is always conserved.

Rule 4: Colour-reversing axes $2'$ or planes m' are conserved by displacements which are perpendicular to the rotation axes or symmetry planes.

Rule 5: An ordinary twofold axis or mirror plane is conserved only by displacements parallel to this axis or plane of symmetry.

The displacements conserving symmetry elements of order greater than 2 (*i.e.* $3,4,6,\bar{3},\bar{4},\bar{6},4',6',\bar{3}',\bar{4}',\bar{6}'$; the threefold colour-reversing axis is not included since $3'=31'$) are determined by combining (1) and (2) as indicated above. For such symmetry elements we have the following rules; the first of these rules may be regarded as a generalization of rule 5.

Rule 6: An ordinary n-fold rotation axis ($n=2,3,4,6$) or mirror plane is conserved only by displacements parallel to this axis or plane of symmetry.

Rule 7: Colour-reversing $\bar{3}'$, $\bar{4}'$, $\bar{6}'$ rotoinversion axes are conserved only by displacements along the axis.

Rule 8: The ordinary rotoinversion axes $\bar{3},\bar{4},\bar{6}$ and the colour-reversing rotation axes $4'$, $6'$ are destroyed by any displacement.

3. Part II: Variation of the spatial symmetry*

In this part we investigate how the relative displacement changes the symmetry of periodic composites. The components of such a composite are necessarily periodic, and in this part they are considered to have three-dimensional translational symmetry. However, this attitude by no means restricts the proposed treatment which can identically be applied for composites formed by two components of one- or two-dimensional periodicity.

The presence of translational symmetry in a dichromatic composite has two important consequences. First of all, the spatial group of the composite before or after displacement may be either symmorphic or nonsymmorphic. Thus, some of the symmetry elements of the composite may be screw axes or glide-reflection planes (see § 3.3). Secondly, unlike the point-symmetry variation, there exist displacements which conserve the original composite.

3.1. *Displacements conserving a periodic composite*

The displacements which leave the original periodic composite unchanged may be classified into two categories, namely:

* From hereon we use the terms 'spatial symmetry' and 'spatial group' to signify that the translational symmetry present may be one, two or three dimensional, and reserve the terms 'space symmetry' and 'space group' for three-dimensional cases.

(i) displacements due to the periodicity of the components; and

(ii) displacements due to the periodicity of the composite.

As mentioned above, the components of a periodic composite always have translational symmetry. The translation group of the Bravais lattice of each component contains, by definition, all the displacement vectors for which the component is invariant in space. Thus, if the relative displacement of the black (white) component is equal to a translation vector of the black (white) lattice, then the composite is recreated at its original position. Displacements of this category are termed 'composite repeat displacements' and they join points of the same colour in the dichromatic composite.

The second category of displacements is related to periodic composites with a misorientation relationship which yields a coincidence site lattice (CSL) (see, for example, Grimmer, Bollmann & Warrington, 1974). The latter is a sublattice common to both components generated by the set of neutral sites in the dichromatic composite. In such cases there are antitranslation vectors, *i.e.* vectors joining white to black sites, which reconstruct the composite as a whole. If the black component is displaced by any antitranslation vector, the original composite is recreated but, in general, has its neutral origin located at a new position. The shift of the CSL is equal to a translation vector of the white component.

As an illustration of displacements of the second category we consider a dichromatic pattern† formed by rotating a black face-centred cubic lattice by an angle $\theta=36.9°$ along [001] with respect to an identical white lattice (Fig. 3). This misorientation corresponds

† A dichromatic pattern is a special composite and is defined by Pond & Bollmann (1979) as the composite consisting of two interpenetrating Bravais lattices.

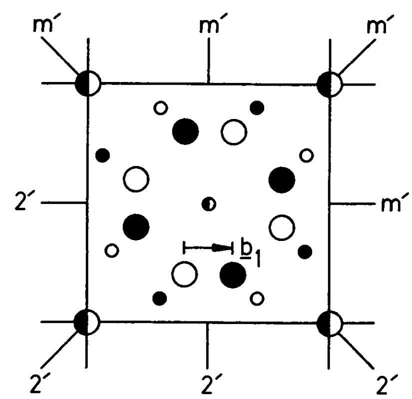

Fig. 3. Projection along [001] of the CSL dichromatic pattern formed by face-centred cubic lattices with misorientation [001]/36.9°. The size of the symbols represents the . . . *ABABA* . . . stacking along [001]; large and small circles represent sites at levels 0 (or 1) and $\frac{1}{2}$ along [001], respectively. Open and filled circles indicate the white and black lattice sites, respectively.

to a CSL with $\Sigma = 5$. Now, if we displace the black lattice by, say, $b_1 = \frac{1}{10}a[310]_w$ (where the subscript refers to the coordinate system of the white lattice), the original composite is reconstructed but its origin is shifted by the translation vector $\frac{1}{2}[110]$ of the white lattice.

3.2. *Displacement vector set*

The effect of relative displacements on the spatial symmetry of a dichromatic composite can be represented in a comprehensive way by means of the vector space (Buerger, 1950). For the purpose of our investigation the vector space is considered as the space containing the displacement vector set of the associated dichromatic composite.

The vector set is formed by drawing vectors between all points in the periodic dichromatic composite. These vectors are then assembled at common origin and the unit cell of the periodic vector set is established. The unit translations of the vector set correspond to the shortest independent displacements which recreate the original composite (it is possible that such displacements reconstruct the original composite in a new position, but this is not important as far as its symmetry is concerned). In other words, the translational symmetry of the vector set represents the periodicity of the spatial symmetry variation. Consequently, it is adequate to investigate changes of the spatial symmetry only for displacements which fall within the Wigner–Seitz cell of the associated vector set. Such displacements are referred to as 'reduced displacements' (Pond & Bollmann, 1979) and denoted $\mathbf{t}'$.

It is evident, from the construction of the vector set, that the fundamental and vector sets have an equal number of translational axes. In the case of dichromatic composites with no translational symmetry the vector set is aperiodic and, hence, no restrictions are imposed on the displacements. For composites with one- or two-dimensional periodicity the unit cell of the vector set is linear or planar respectively and the reduced displacements must be projected within the corresponding Wigner–Seitz cell. Finally, three-dimensional periodicity in a composite implies a three-dimensional Wigner–Seitz cell and, thus, the reduced displacements must end within or at the boundaries of this cell.

3.3. *General and special displacements*

The spatial group of a periodic composite may be symmorphic or nonsymmorphic. The symmetry elements of the former are equivalent to point symmetry elements and their conservation rules have already been studied in part I. It remains, therefore, to deal with translation-coupled symmetry elements which may be present in the original composite or be created by the appropriate displacement of the black component. Consider, for example, the one-dimensional periodic composite in Fig. 4(*a*). The Wigner–Seitz cell of the associated vector set is along the translation axis and extends from $-\mathbf{a}/2$ to $\mathbf{a}/2$. Any infinitely small displacement of the black component away from the reference position destroys the mirror plane m'_y of the original composite. Thus, for $-\mathbf{a}/2 < \mathbf{t}' < \mathbf{a}/2$ and $\mathbf{t}' \neq \mathbf{0}$ the mirror m'_y is not present in the obtained dichromatic composite. The displacements $\mathbf{t}' = \pm\mathbf{a}/2$, however, bring the two components in a glide-reflection relationship (Fig. 4*b*).

The variation of spatial symmetry of a periodic composite is, therefore, a consequence of two reasons. Firstly, the displacement may destroy some symmetry elements of the original composite. Secondly, the same displacement may transform some (if not all) translation-free rotation axes or mirror planes of the original composite into screw axes or glide planes (or *vice versa*). Displacements with this property, as well as displacements which conserve the composite as a whole, will be called 'special displacements', whereas the remaining are referred to as 'general displacements'.

Special displacements correspond to dichromatic composites in which the relative translational position of their components is defined by a vector of specific magnitude; the end-points of such vectors are special positions in the Wigner–Seitz cell of the associated vector set. Any infinitely small deviation away from the special position changes the symmetry of the composite. General displacements, on the other hand, are associated with dichromatic composites, the symmetry of which remains unchanged over wide limits of displacement.

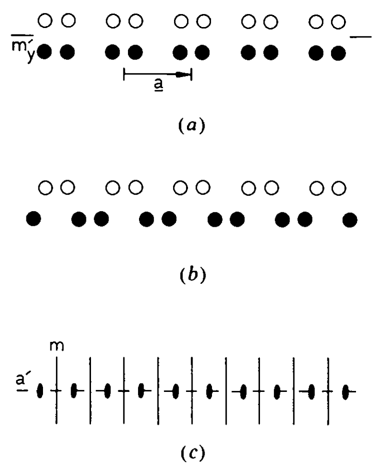

Fig. 4. (*a*) A composite with one-dimensional periodicity; the unit translation is indicated by the vector $\mathbf{a}$. Open and filled circles represent points of the white and black (one-dimensional) components respectively. The composite exhibits symmetry $\not{p}mm'2'$. (*b*) The composite obtained from (*a*) by displacing the black component by $\mathbf{t} = \mathbf{a}/2$; its symmetry is $\not{p}ma'2'$. (*c*) The disposal of symmetry elements for the composite shown in (*b*).

Table 5. *Possibilities of symmetry-element conservation in spatial symmetry variation*

The symbols have the following meaning: *tf* = translation-free symmetry element, *tb* = translation-bearing symmetry element.

		Type of symmetry element	
No.	Kind of symmetry element	Before displacement	After displacement
1	Ordinary	*tf*	*tf*
2		*tb*	*tb*
3	Colour-reversing	*tf*	*tf*
4		*tf*	*tb*
5		*tb*	*tb*
6		*tb*	*tf*

3.4. *Conservation of translation-coupled symmetry elements*

Both general and special displacements change the spatial symmetry of the dichromatic composite by destroying some symmetry elements originally present while conserving others. By conservation of an ordinary or colour-reversing symmetry element we understand either that the element is invariant by the displacement or that the relative shift of the components transforms the symmorphic element into a nonsymmorphic one or *vice versa.* However, since a displacement changes only the relative translational position of the two components, a special displacement transforms only colour-reversing axes and/or mirror planes to their respective translation-coupled counterparts or *vice versa.*

The various cases of symmetry-operation conservation are given in Table 5. Cases 1 and 3 have already been investigated in part I. Moreover, it can easily be seen that in cases 2 and 5 the conditions for conservation of the associated symmetry operations are identical to those for symmorphic operations. We have, therefore, to consider only cases 4 and 6 here. For the former, let $S_c \equiv (S_c|\mathbf{0})$ be the symmetry operation of the original composite and let $(S_c|\boldsymbol{\tau})$ be the Seitz symbol (Seitz, 1936) of the corresponding nonsymmorphic operation created by the displacement $\mathbf{t}'$. Then, in the original composite there is at least a white and a black point, $\mathbf{r}_w$ and $\mathbf{r}_b$, respectively, for which $S_c\mathbf{r}_w \equiv (S_c|\mathbf{0})\mathbf{r}_w = \mathbf{r}_b$. The positions of the above points, after displacement $\mathbf{t}'$, are $\mathbf{r}_w - \mathbf{t}'/2$ and $\mathbf{r}_b + \mathbf{t}'/2$ and their symmetry relationship is $(S_c|\boldsymbol{\tau})(\mathbf{r}_w - \mathbf{t}'/2) \equiv S_c(\mathbf{r}_w - \mathbf{t}'/2) + \boldsymbol{\tau} = \mathbf{r}_b + \mathbf{t}'/2$. A symmorphic colour-reversing symmetry operation S_c is, therefore, transformed to its nonsymmorphic equivalent $(S_c|\boldsymbol{\tau})$ only by displacements satisfying the relation

$$S_c(-\mathbf{t}'/2) + \boldsymbol{\tau} = \mathbf{t}'/2. \qquad (3)$$

Similarly, a nonsymmorphic colour-reversing operation $(S_c|\boldsymbol{\tau})$ is transformed to its symmorphic residue by displacements given by

$$S_c(-\mathbf{t}'/2) - \boldsymbol{\tau} = \mathbf{t}'/2. \qquad (4)$$

We are now ready to establish the conditions for conservation of nonsymmorphic symmetry elements. Ordinary or colour-reversing translation-coupled elements are invariant by exactly the same displacements which conserve the corresponding symmorphic elements. A colour-reversing glide-reflection plane, for example, is conserved by displacements perpendicular to it irrespectively of its translation component (*cf.* rule 4). Thus, it can be said that rules 1–8 given in part I are identically applied for the invariance of symmorphic and nonsymmorphic symmetry elements. This is demonstrated by considering the following example. The dichromatic composite in Fig. 4(*b*) has spatial symmetry $\not{p}ma'2'$, where $\not{p}$ stands for the one-dimensional lattice and the disposal of the symmetry elements is shown in Fig. 4(*c*). A displacement $\mathbf{t}'$ perpendicular to the a' conserves this colour-reversing glide-reflection plane as well as the ordinary plane m. Conversely, if the displacement is parallel to a', and hence perpendicular to m, both symmetry planes are destroyed.

We examine next the conditions under which a symmorphic symmetry element is transformed to a nonsymmorphic one or *vice versa.* Consider, for example, a twofold colour-reversing axis along the z axis of a right-handed orthogonal coordinate system of the white component. The considered $2'$ axis can be changed to only a $2_1'$ screw axis parallel to the z direction of the coordinate system. Thus, we have $2_1' \equiv (2'|00c/2)$, where c is the magnitude of the periodicity vector along the z axis. Consequently, the displacements transforming $2'$ to $2_1'$ are given by

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -t_x'/2 \\ -t_y'/2 \\ -t_z'/2 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ c/2 \end{pmatrix} = \begin{pmatrix} t_x'/2 \\ t_y'/2 \\ t_z'/2 \end{pmatrix},$$

i.e. by $\mathbf{t}' = (x, y, c/2)$. This can be written as $\mathbf{t}' = (x, y, 0) + (0, 0, c/2)$, where the first term corresponds to a displacement for which the initial $2'$ axis is invariant and the second term is the displacement bringing the two components into $2_1'$ relationship.

Rule 9: Colour-reversing screw diads or glide-reflection planes are created from $2'$ axes or m' planes (or *vice versa*) by displacements $\mathbf{t}' = \mathbf{t}_1' + \mathbf{t}_2'$, where $\mathbf{t}_1'$ is the displacement leaving the $2'$ or m' invariant and $\mathbf{t}_2'$ is a displacement component parallel to these symmetry elements and equal to the translation part of the screw diad or glide plane.

For n-fold screw axes ($n > 2$) we note that the relative displacement simply shifts one component with respect to the other.

Rule 10: Only four and sixfold colour-reversing rotation axes can be changed to screw axes or *vice versa.* The screw axes have neither right nor left sense, *i.e.* they can be only $4_2'$ and $6_3'$, and they correspond to a relative displacement parallel to the original axis with magnitude equal to half the period along the colour-reversing $4'$ and $6'$ axes.

As was pointed out above, any displacement changes the spatial and/or point symmetry of the original dichromatic composite. The point-symmetry case was investigated in part I, and remains, therefore, to give the procedure for the determination of the spatial symmetry variation. The method is based on: (*a*) the original composite exhibits the highest possible symmetry for the given components and misorientation relationship, and (*b*) a displacement can never modify the periodicity of the dichromatic composite (Pond & Vlachavas, 1983). This means that the spatial symmetry group of the composite with $\mathbf{t}\neq\mathbf{0}$ must be a subgroup of that corresponding to $\mathbf{t}=\mathbf{0}$ but the two groups have the same translational subgroups.

3.5. *Determination of the spatial symmetry for general displacements*

According to the discussion in the foregoing section, general displacements can never transform a symmorphic symmetry element into a nonsymmorphic one or *vice versa.* The spatial symmetry of a composite obtained by a general displacement is, thus, described by a group in which: (i) all symmetry operations are also symmetry operations of the original composite, and (ii) the subgroup of translations is the same as that of the original composite. General displacements correspond, therefore, to spatial subgroups in which the descent in symmetry has only affected the symmorphic or nonsymmorphic rotations and reflections but not the accompanying translations in the unit cell. In other words, the spatial symmetry for general displacements is a *zellengleiche* subgroup (Hermann, 1929) of the original symmetry group. Thus, the procedure to determine the spatial symmetry for general displacements is as follows.

Let G be the spatial symmetry of the original composite and g be its point group. Firstly, we investigate the point-symmetry variation by the method proposed in part I. This allows us to establish the displacements conserving subgroups of the point group g. Secondly, we obtain the list of *zellengleichen* subgroups of G. Hermann (1929) has shown that there is only one *zellengleiche* subgroup of G for each subgroup of g. Thus, if the displacement conserving a particular subgroup of g is obtained, then this displacement conserves also the isomorphic *zellengleiche* subgroup. In most cases the answer can be written immediately by inspection of the symbols. However, attention should be given for the cases where the point subgroup adopts crystallographically non-equivalent orientations in the point group of the original composite. In such cases different *zellengleichen* subgroups may correspond to the non-equivalent point groups. The ambiguity can be resolved by considering the point symmetry operations that are conserved by the particular general displacement. Thus, we can establish the point subgroups, and consequently the *zellengleichen* subgroups, corresponding to these displacements.

3.6. *Determination of the spatial symmetry for special displacements*

Special displacements give dichromatic composites with spatial symmetry described by a group which: (i) has the same subgroup of translations as the original composite; (ii) is isomorphous with a subgroup of the point group of the original composite; and (iii) may contain translation-coupled colour-reversing symmetry elements corresponding to translation-free colour-reversing elements present originally in the composite or *vice versa.* Consequently, a composite corresponding to a special displacement displays nonsymmorphic/symmorphic symmetry isomorphic to the symmorphic/nonsymmorphic symmetry of a *zellengleiche* subgroup of the original composite. This can be expressed by the following considerations.

Let G be the spatial group of the original composite, T the translation group of the Bravais lattice of G and G_z a *zellengleiche subgroup of* G. Then, G_z can be expressed as the sum of the left cosets of its translation group T:

$$G_z=(r_1|\boldsymbol{\tau}_1)T+(r_2|\boldsymbol{\tau}_2)T+\ldots+(r_h|\boldsymbol{\tau}_h)T$$
$$+(r'_{h+1}|\boldsymbol{\tau}_{h+1})T+(r'_{h+2}|\boldsymbol{\tau}_{h+2})T+\ldots+(r'_{2h}|\boldsymbol{\tau}_{2h})T,$$

where $\boldsymbol{\tau}_i$ is the supplementary displacement associated with the translation-coupled point symmetry operation r_i and the rotational parts $r_1, r_2, \ldots, r_h, r'_{h+1}, r'_{h+2}, \ldots, r'_{2h}$ form the point group g_z isomorphic to G_z. A special displacement $\mathbf{t}'$ will change $\boldsymbol{\tau}_{h+i}$ to $\boldsymbol{\tau}_{h+i}+\boldsymbol{t}'$ so that G_z changes to

$$G_s=(r_1|\boldsymbol{\tau}_1)T+(r_2|\boldsymbol{\tau}_2)T+\ldots+(r_h|\boldsymbol{\tau}_h)T$$
$$+(r'_{h+1}|\boldsymbol{\tau}_{h+1}+\mathbf{t}')T+(r'_{h+2}|\boldsymbol{\tau}_{h+2}+\mathbf{t}')T$$
$$+\ldots+(r'_{2h}|\boldsymbol{\tau}_{2h}+\mathbf{t}')T.$$

To establish the spatial groups for special displacements we apply, therefore, the following algorithm. For each *zellengleiche* subgroup G_z of the original group we determine the isomorphic spatial groups having the same Bravais lattice as G_z and the same ordinary symmetry operations. For each of the so obtained spatial groups G_s we check if there is a displacement $\mathbf{t}'$ to transform G_z to G_s. This can be achieved by adopting the description of a spatial group by means of its 'general positions' (*International Tables for X-ray Crystallography*, 1965). Comparison between the sets of general positions of G_z and G_s will yield the required displacement $\mathbf{t}'$.

We consider, as an example, the two-dimensional group $p2'm'm$; the general positions of this group are: x, y; $x, \bar{y}$; $\bar{x}', y'$; $\bar{x}', \bar{y}'$, where the primes indicate that in the particular general position colour-reversing occurs. The two-dimensional space groups in the class $2'm'm$ are: $p2'm'm$, $p2'm'g$, $p2'g'm$ and $p2'g'g$ (Belov & Tarhkova, 1956). We note, however, that both $p2'm'g$ and $p2'g'g$ possess an ordinary g plane which is not present in the original group $p2'm'm$. Thus, only the group $p2'g'm$ may correspond to a special displacement. Its general positions are expressed relative to the coordinate system of the original group as x,y; $x,\bar{y}$; $\bar{x}', \frac{1}{2}+y'$; $\bar{x}', \frac{1}{2}-y'$. The first and second positions in both sets correspond to the common ordinary elements of $p2'm'm$ and $p2'g'm$. Consequently, we can transform $p2'm'm$ to $p2'g'm$ by the displacement $\mathbf{t}' = (0, \frac{1}{2})$ as can be seen by considering the geometric representations of the two groups (Fig. 5).

3.7. *Example of spatial symmetry variation*

To conclude this paper the procedure for studying the symmetry variation of a periodic composite is demonstrated by the following example. The original composite considered is formed by two face-centred cubic lattices of identical lattice parameter **a** which are related by the misorientation relationship [001]/36.9° (Fig. 3). As was mentioned in § 3.1, this composite corresponds to the $\Sigma = 5$ CSL misorientation, its space group is $I4/mm'm'$, and its vector set has a body-centred tetragonal unit cell with lattice parameters, expressed relative to the white lattice, $\mathbf{b}_1 = \frac{1}{10}a[310]_w$, $\mathbf{b}_2 = \frac{1}{10}a[1\bar{3}0]_w$ and $\mathbf{b}_3 = \mathbf{b}_1 \times \mathbf{b}_2 = [001]_w$. The coordinate system used for expressing the displacements $\mathbf{t}'$ is as follows: the origin is taken to be a coincidence site, and the unit vectors along the x, y and z axes are $\mathbf{b}_1$, $\mathbf{b}_2$ and $\mathbf{b}_3$, respectively.

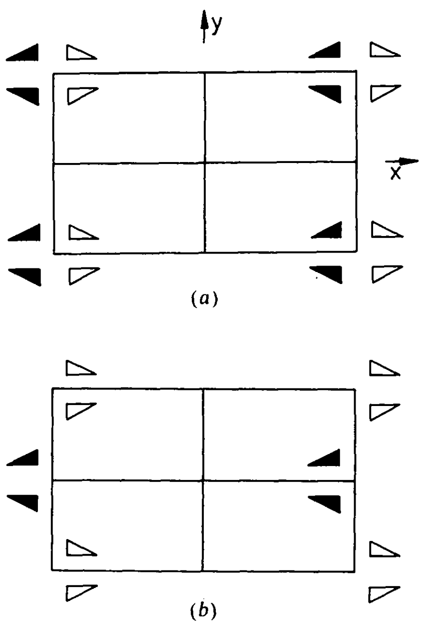

Fig. 5. Geometrical representations of (*a*) $p2'm'm$ and (*b*) $p2'g'm$ two-dimensional space groups.

Table 6. *Zellengleichen subgroups of the two-coloured space group $I4/mm'm'$*

The serial numbers in this table correspond to those in Table 1.

No.	*Zellengleiche* subgroup	No.	*Zellengleiche* subgroup
1	$I4/mm'm'$	18	$C2'/m'$
2	$I\bar{4}2'm'$	19	$C2/m$
3	$I\bar{4}2'm'$	20	$Im'm'2$
4	$I4m'm'$	21	$Fm'm'2$
5	$I42'2'$	22	$I2'2'2$
6	$I4/m$	23	$F2'2'2$
7	$I\bar{4}$	24	$P\bar{1}$
8	$I4$	25	Cm'
9	$Im'm'm$	26	Cm'
10	$Fm'm'm$	27	Cm'
11	$Im'm2'$	28	Cm'
12	$Im'm2'$	29	$C2'$
13	$Fm'm2'$	30	$C2'$
14	$Fm'm2'$	31	$C2'$
15	$C2'/m'$	32	$C2'$
16	$C2'/m'$	33	Cm
17	$C2'/m'$	34	$C2$
		35	$P1$

(*a*) *General displacements*: the point-symmetry variation of $4/mm'm'$ has already been studied in § 2.4 and, hence, Table 4 may be regarded as giving the point symmetry of the composites obtained by general displacements. In order to establish the space symmetry of these composites we consider the list of the *zellengleichen* subgroups of $I4/mm'm'$ (Table 6) and we combine this list with Table 4 (see § 3.5). Consider, for example, the displacement $\mathbf{t}' = (0, 0, z)$ which yields a composite with point symmetry $42'2'$. Referring to Table 6 we see that the *zellengleiche* subgroup of $I4/mm'm'$ belonging to the class $42'2'$ is $I42'2'$ and, consequently, the space group of the composite obtained by $\mathbf{t}' = (0, 0, z)$ is $I42'2'$.

This procedure may lead to ambiguity when a point subgroup adopts crystallographically non-equivalent orientations in the point group of the original composite. However, the ambiguity can easily be resolved as explained in § 3.5. Such a case occurs for the displacements $\mathbf{t}' = (x, 0, 0)$ and $\mathbf{t}' = (x, x, 0)$; both of them correspond to composites with point symmetry $m'm2'$. The subgroup $m'm2'$ adopts four different orientations in $4/mm'm'$ located over an angle 45° about the fourfold axis; two of these orientations are not crystallographically equivalent. To establish, therefore, the space groups of the composites with $\mathbf{t}' = (x, 0, 0)$ and $\mathbf{t}' = (x, x, 0)$ we note that the first displacement conserves the subgroup $m'm2' = \{1, 2_{010}^{1'}, s_{001}, s'_{100}\}$ and, according to Table 6, the respective space group is $Im'm2'$. On the other hand, if the displacement $\mathbf{t}' = (x, x, 0)$ is considered, then the conserved symmetry operations form the subgroup $m'm2' = \{1, 2_{\bar{1}10}^{1'}, s_{001}, s'_{110}\}$ and, hence, the space group for $\mathbf{t}' = (x, x, 0)$ is $Fm'm2'$.

In a similar way we determine the space symmetry for the remaining displacements. However, we must remember at this point that the symmetry of a composite varies periodically with the displacement. Thus, $\mathbf{t}'$ and $\mathbf{t}'+\mathbf{t}_{vs}$, where $\mathbf{t}_{vs}$ is a translational vector of the vector set associated with the original composite, will yield the same composites. The shortest $\mathbf{t}_{vs}$ is $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ and this vector, or one of its symmetry equivalents, must be added to each displacement determined above in order to obtain the full set of general displacements within the Wigner–Seitz cell.

(*b*) *Special displacements*: first of all, we establish by the algorithm mentioned in § 3.6 the space groups which may correspond to special displacements (Table 7). We must notice, however, that the space groups are indicated in Table 7 by their standard symbols, and that different settings may be possible. Thus, for the group $Imm'a'$ the glide-reflection plane may be perpendicular to either the x axis or the y axis of the coordinate system of the original composite; thus, we have either $Ib'm'm$ or $Im'a'm$ (see *International Tables for X-ray Crystallography*, 1965). To determine the displacement transforming $Im'm'm$ to, say, $Im'a'm$ we consider the general positions of both groups:

$Im'm'm$: $(0, 0, 0; \frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$

$$\begin{array}{cccc}
(1|000) & (2^{1}_{001}|000) & (\bar{1}|000) & (s_{001}|000) \\
x, y, z & \bar{x}, \bar{y}, z & \bar{x}, \bar{y}, \bar{z} & x, y, \bar{z} \\
(2^{1'}_{100}|000) & (2^{1'}_{010}|000) & (s'_{100}|000) & (s'_{010}|000) \\
x', \bar{y}', \bar{z}' & \bar{x}', \bar{y}, \bar{z}' & \bar{x}', y', z' & x', \bar{y}, z'
\end{array}$$

and

$Im'a'm$: $(0, 0, 0; \frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$

$$\begin{array}{cccc}
(1|000) & (2^{1}_{001}|000) & (\bar{1}|000) & (s_{001}|000) \\
x, y, z & \bar{x}, \bar{y}, z & \bar{x}, \bar{y}, \bar{z} & x, y, \bar{z} \\
(2^{1'}_{100}|\frac{1}{2}00) & (2^{1'}_{010}|\frac{1}{2}00) & (s'_{100}|\frac{1}{2}00) & (s'_{010}|\frac{1}{2}00) \\
\frac{1}{2}+x', \bar{y}', \bar{z}' & \frac{1}{2}-x', y', \bar{z}' & \frac{1}{2}-x', y', z' & \frac{1}{2}+x', \bar{y}', z'.
\end{array}$$

The general positions of the first line in the two groups correspond to their common symmetry operations. $Im'm'm$ is, therefore, transformed to $Im'a'm$ by $\mathbf{t}'=(\frac{1}{2}, 0, 0)$ or $\mathbf{t}'=(0, \frac{1}{2}, \frac{1}{2})$. On the other hand, the general positions of $Ib'm'm$ are

$Ib'm'm$: $(0, 0, 0; \frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$

$$\begin{array}{cccc}
(1|000) & (2^{1}_{001}|000) & (\bar{1}|000) & (s_{001}|000) \\
x, y, z & \bar{x}, \bar{y}, z & \bar{x}, \bar{y}, \bar{z} & x, y, \bar{z} \\
(2^{1'}_{100}|0\frac{1}{2}0) & (2^{1'}_{010}|0\frac{1}{2}0) & (s'_{100}|0\frac{1}{2}0) & (s'_{010}|0\frac{1}{2}0) \\
x', \frac{1}{2}-y', \bar{z}' & \bar{x}', \frac{1}{2}+y', \bar{z}' & \bar{x}', \frac{1}{2}+y', z' & x', \frac{1}{2}-y', z'
\end{array}$$

and, consequently, this group corresponds to $\mathbf{t}'=(0, 1/2, 0)$ or $\mathbf{t}'=(1/2, 0, 1/2)$.

As can be seen from Table 7 a composite with symmetry, say, $I4/mc'm'$ is created by $\mathbf{t}'=(0, 0, \frac{1}{2})$ or $\mathbf{t}'=(\frac{1}{2}, \frac{1}{2}, 0)$. These two displacements are, however, related by a translation operator of the vector set associated with the original composite, *i.e.* $(0, 0, \frac{1}{2})=(\frac{1}{2}, \frac{1}{2}, 0)+(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. This is an immediate consequence of the fact that the translational symmetry of the vector set represents, as explained in § 3.2, the periodicity of the spacial symmetry variation.

The space-symmetry variation of the composite $I4/mm'm'$ is summarized in Table 8. In the heading of the first column of this table the symbol (0, 0, 0;

Table 7. *Determination of the space groups corresponding to special displacements for the group $I4/mm'm'$*

The coordinate system for specifying $\mathbf{t}'$ is as follows: the origin is taken to be the centre of the Wigner–Seitz cell of the associated vector set, x is parallel to $\mathbf{b}_1$, y to $\mathbf{b}_2$ and z to $\mathbf{b}_1 \times \mathbf{b}_2$.

Zellengleiche subgroup G_z	Isomorphic space group for special displacement G_s	Fractional coordinates of displacements $\mathbf{t}'$ transforming G_z to G_s
$I4/mm'm'$	$I4/mc'm'$	$(0, 0, \frac{1}{2}), (\frac{1}{2}, \frac{1}{2}, 0)$
$I\bar{4}2'm'$	$I\bar{4}2'd'$	$(\frac{1}{2}, 0, \frac{1}{4}), (0, \frac{1}{2}, \frac{1}{4})$, $(0, \frac{1}{2}, -\frac{1}{4}), (\frac{1}{2}, 0, -\frac{1}{4})$
$I4m'm'$	$I4c'm'$	$(0, 0, \frac{1}{2}), (\frac{1}{2}, \frac{1}{2}, 0)$
$Im'm'm$	$Ib'a'm$	$(0, 0, \frac{1}{2}), (\frac{1}{2}, \frac{1}{2}, 0)$,
$Im'm'm$	$Imm'a'$	$(\frac{1}{2}, 0, 0), (0, \frac{1}{2}, 0)$ $(0, \frac{1}{2}, \frac{1}{2}), (\frac{1}{2}, 0, \frac{1}{2})$
$Im'm2'$	$Ima'2'$	$(\frac{1}{2}, 0, 0), (0, \frac{1}{2}, 0)$, $(0, \frac{1}{2}, \frac{1}{2}), (\frac{1}{2}, 0, \frac{1}{2})$
$C2'/m'$	$C2'/c'$	$(0, 0, \frac{1}{2}), (\frac{1}{2}, \frac{1}{2}, 0)$
$Im'm'2$	$Ib'a'2$	$(0, 0, \frac{1}{2}), (\frac{1}{2}, \frac{1}{2}, 0)$
$Im'm'2$	$Im'a'2$	$(\frac{1}{2}, 0, 0), (0, \frac{1}{2}, 0)$, $(0, \frac{1}{2}, \frac{1}{2}), (\frac{1}{2}, 0, \frac{1}{2})$
$Fm'm'2$	$Fd'd'2$	$(\frac{1}{2}, 0, \frac{1}{4}), (0, \frac{1}{2}, \frac{1}{4})$, $(0, \frac{1}{2}, -\frac{1}{4}), (\frac{1}{2}, 0, -\frac{1}{4})$
Cm'	Cc'	$(0, 0, \frac{1}{2}), (\frac{1}{2}, \frac{1}{2}, 0)$

Table 8. *Variation of the dichromatic composite symmetry $I4/mm'm'$ with relative displacement $\mathbf{t}'$*

The coordinate system used for expressing $\mathbf{t}'$ is the same as that in Table 7.

Fractional coordinates of equivalent displacements $(0, 0, 0; \frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$	Rank	Space symmetry
$(0, 0, 0)$	2	$I4/mm'm'$
$(0, 0, \frac{1}{2})$	2	$I4/mc'm'$
$(\frac{1}{2}, 0, \frac{1}{4}), (0, \frac{1}{2}, \frac{1}{4})$	4	$I\bar{4}2'd'$
$(\frac{1}{2}, 0, 0), (0, \frac{1}{2}, 0)$	4	$Imm'a'$
$(0, 0, z), (0, 0, \bar{z})$	4	$I42'2'$
$(x, 0, 0), (0, x, 0), (\bar{x}, 0, 0), (0, \bar{x}, 0)$	8	$Im'm2'$
$(x, x, 0), (\bar{x}, x, 0), (x, \bar{x}, 0), (\bar{x}, x, 0)$	8	$Fm'm2'$
$(x, 0, z), (0, x, z), (\bar{x}, 0, z), (0, \bar{x}, z)$, $(x, 0, \bar{z}), (0, x, \bar{z}), (\bar{x}, 0, \bar{z}), (0, \bar{x}, \bar{z})$	16	$C2'$
$(x, x, z), (\bar{x}, x, z), (x, \bar{x}, z), (\bar{x}, \bar{x}, z)$, $(x, x, \bar{z}), (\bar{x}, x, \bar{z}), (x, \bar{x}, \bar{z}), (\bar{x}, \bar{x}, \bar{z})$	16	$C2'$
$(x, y, 0), (y, x, 0), (x, \bar{y}, 0), (y, \bar{x}, 0)$, $(\bar{x}, \bar{y}, 0), (\bar{y}, \bar{x}, 0), (\bar{x}, y, 0), (\bar{y}, x, 0)$	16	Cm
$(x, y, z), (\bar{x}, y, z), (x, \bar{y}, z), (\bar{x}, \bar{y}, z)$, $(y, x, z), (\bar{y}, x, z), (y, \bar{x}, z), (\bar{y}, \bar{x}, z)$, $(x, y, \bar{z}), (\bar{x}, y, \bar{z}), (x, \bar{y}, \bar{z}), (\bar{x}, \bar{y}, \bar{z})$, $(y, x, \bar{z}), (\bar{y}, x, \bar{z}), (y, \bar{x}, \bar{z}), (\bar{y}, \bar{x}, \bar{z})$	32	$P1$

$\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$ appears. This means that the full set of displacements corresponding to a particular composite symmetry is obtained by adding the vector $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ in turn to all displacements of the set given in the first column. The full set of displacements contains all the vectors whose end-points are equivalent positions in the space group of the vector set associated with the original composite. Such a set of displacements will be referred to as 'set of equivalent displacements' and the number of equivalent displacements in the set is called its rank.

In part I we pointed out there are displacements which create symmetry-related composites. This is true for periodic composites as well. In this case, however, the periodicity of the spatial symmetry variation must also be taken into account. If the translational symmetry of the vector set of a periodic composite is described by a primitive lattice, then the set of equivalent displacements contains all the shift vectors which yield symmetry-related composites. On the other hand, for vector sets with non-primitive lattices the set of equivalent displacements contains in addition displacements which are associated with identical composites. This is the case for the above-considered example. The equivalent displacements $(0, 0, z)$, $(0, 0, \bar{z})$, $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}+z)$, $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}-z)$, for instance, yield composites with symmetry $I42'2'$. But all these composites are not symmetry equivalent. The first and third, as well as the second and fourth, displacements are interrelated by the translation vector $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ of the vector set and, hence, they correspond to identical composites. Thus, the number of symmetry-related composites depends on whether the lattice of the vector set (or, equivalently, of the periodic composite; see Buerger, 1959) is primitive or not. The number of symmetry-related composites is equal to the rank of the set of equivalent displacements divided by the number of lattice points in the unit cell of the periodic composite. This can be expressed comprehensively through a detailed study of the symmetry-related composites obtained by general and special displacements. Such a formulation in group theoretical terms will, however, be discussed in a following paper.

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Composite Symmetry Formed by Two Identical Point Groups With Common Origin

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Abstract

A group-theoretical method is presented that enables the derivation of the symmetry of any composite created by the superposition of two identical point groups. The invariant points of the two components are considered in coincidence and the composite symmetry is expressed as the intersection of two sets of symmetry operations. The first set contains the symmetry operations common in the components when their mutual disposition is taken into account, whereas in the second set belong the additional

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